

Fermi-edge singularity in the vicinity of the resonant scattering condition

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Fermi-edge absorption theory predicting the spectrum, $A(\omega) \propto \omega^{-2\delta_0/\pi + \delta_0^2/\pi^2}$, relies on the assumption that scattering phase, δ_0 , is frequency-independent. Dependence of δ_0 on ω becomes crucial near the resonant condition, where the phase changes abruptly by π . In this limit, due to finite time spent by electron on a resonant level, the scattering is *dynamic*. We incorporate this time delay into the theory, solve the Dyson equation with a modified kernel and find that, near the resonance, $A(\omega)$ behaves as $\omega^{-3/4} |\ln \omega|$. Resonant scattering off the core hole takes place in 1D and 2D in the presence of an empty subband above the Fermi level; then attraction to hole splits off a resonant level from the bottom of the empty subband. Fermi-edge absorption in the regime when resonant level transforms into a Kondo peak is discussed.

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Introduction. Many-body character of absorption from the localized level into continuum in the presence of the Fermi sea [1] manifests itself via two mechanisms: scattering of the excited electron from the hole left behind and adjustment of the Fermi sea to the abrupt switch-on of the hole potential. Correspondingly, near the threshold, the spectrum, $A(\omega) = I(\omega)P(\omega)$, is a product [2] of two functions

$$I(\omega) = \left(\frac{D}{\omega}\right)^{2\delta_0/\pi}, \quad P(\omega) = \left(\frac{D}{\omega}\right)^{-\delta_0^2/\pi^2}, \quad (1)$$

where D is the bandwidth; δ_0 is the phase shift for s -scattering. Phase δ_0 is related to the hole potential strength V as $\tan \delta_0 = \pi \nu_0 V$, where ν_0 is the density of states. The function $I(\omega)$ is the single-electron-line contribution, which describes the first mechanism, while $P(\omega)$ accounts for the shake-up effects.

Derivation of Eq. (1) by Nozieres and De Dominicis (ND) in Ref. [2] strongly relies on the assumption that δ_0

is frequency-independent. This assumption implies that the scattering is *instantaneous*. In the present paper we focus on the situation when this assumption is violated. This situation realizes when the Fermi level is close to an empty upper subband, as shown in Fig. 1. In such an arrangement it is important that even a *deep* core-hole creates a localized level a distance E_{ex} below the bottom of the upper subband, see Fig. 1. Formation of a localized level happens in low dimensions (2D and 1D). Experimental and theoretical studies of the arrangement in which Fermi level is near the bottom of empty subband have been reported in [3–6] and [7–13], respectively.

Due to degeneracy with continuum of lower band, the level E_{ex} acquires a finite width, Γ . Then the process underlying the Fermi-edge singularity is not scattering from *bare* core-hole potential but rather resonant scattering on the quasi-local level. Correspondingly, the scattering phase is given by

$$\delta(\omega) = \arctan \frac{\Gamma}{\omega - \Delta}, \quad (2)$$

where Δ is the energy distance from localized level to the Fermi level, E_F . In the limit $\Delta \rightarrow 0$, ω -dependence of δ is strong. Indication that in this limit the ND theory is inapplicable follows from the fact that at $\omega = \Delta$, the phase abruptly changes by π . This, in turn, leads to a paradoxical conclusion that, as Fermi level is swept through the bound state, $I(\omega)$ changes *abruptly* from $I(\omega) \propto 1/\omega$ to $I(\omega) \propto \omega$. By contrast, the shake-up term $P(\omega) \propto \omega^{1/4}$ *does not* experience a jump.

As a resolution of this paradox, in the present paper we show that abrupt change of $I(\omega)$ *does* take place in the frequency interval, $\omega \sim |\Delta|$, which gets *progressively narrow* as Δ goes to 0. We also show that outside this interval, where the ND theory does not apply, a new, *dynamical resonant-scattering* regime governs the absorption [14]. We show that in this regime, instead of Eq. (1), $I(\omega)$ is given by

$$I(\omega) \Big|_{|\Delta| < \omega < \Gamma} = \frac{\nu_0}{2\pi} \frac{\Gamma}{\omega} \ln \left(\frac{E_{ex}}{\omega} \right), \quad (3)$$

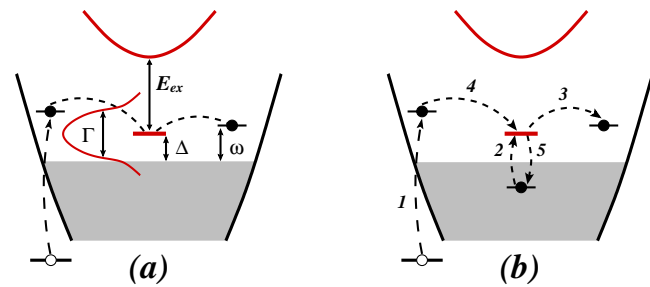


FIG. 1: (Color online) (a): In the vicinity of a topological transition, the core hole potential creates bound state (resonant level) with energy, E_{ex} , measured from the bottom of the upper subband; its lifetime, Γ , is due to a coupling to the lower subband. For a photoelectron with energy, $\omega \ll \Gamma$ above the Fermi level, dynamical character of scattering from resonant level is crucial. (b): Contribution to the absorption amplitude which is strongly affected by resonant character of scattering: two scattering acts involved, (2 + 3) and (4 + 5), have opposite signs of amplitudes, Eq. (10).

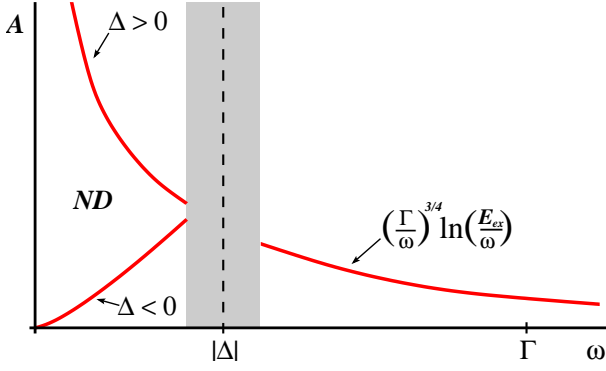


FIG. 2: (Color online) Absorption spectrum, $A(\omega)$, in the situation when the Fermi level is close to resonant level ($|\Delta| \ll \Gamma$) is shown schematically. For $\omega < |\Delta|$ the ω -dependence, Eq. (29), is governed by ND theory. In the "dynamic scattering" domain $|\Delta| < \omega < \Gamma$ the spectrum is $A(\omega) = (\Gamma/\omega)^{3/4} \ln(E_{ex}/\omega) \ln(E_{ex}/\Gamma)$ for any sign of Δ .

independently of the sign of Δ . Our findings are illustrated in Fig. 2.

Dynamic-scattering regime. Within the ND theory, the transient Green function, $\varphi(\tau, \tau'|t, t')$, satisfies the Dyson equation

$$\varphi(\tau, \tau'|t, t') = G(\tau - \tau') + \int_t^{\tau'} d\tilde{\tau} K(\tau, \tilde{\tau}) \varphi(\tilde{\tau}, \tau'|t, t'), \quad (4)$$

where $G(t) = -\nu_0/t$ is the bare electron Green function, and the kernel is defined as $K(\tau, \tilde{\tau}) = VG(\tau - \tilde{\tau})$. The single-electron-line contribution to $A(\omega)$ is expressed in terms of the transient Green function as

$$I(\omega) = -\frac{1}{\pi} \text{Im} \int_{-\infty}^0 dt e^{-i\omega t} \varphi(0^-, t^+|t, 0). \quad (5)$$

Delicate character of Fermi-edge absorption can be inferred from the structure of n -th term,

$$V^n \int_t^0 dt_1 \cdots \int_t^0 dt_n G(-t_1) G(t_1 - t_2) \cdots G(t_n - t), \quad (6)$$

of perturbative expansion of $\varphi(0^-, t^+|t, 0)$ in powers of V , which follows from Eq. (4). It appears that contributions of different orderings of times t_i , Fig. 3a, at which electron is scattered, cancel each other up to $1/n!$.

Frequency dependence of δ leads to a time delay, τ , in the scattering processes, as illustrated in Fig. 3b. Each delay ranges from E_{ex}^{-1} to $|\Delta|^{-1}$. As a result, in the limit $\Delta \rightarrow 0$, the above cancellation is *completely destroyed*. On the quantitative level, dynamical character of the resonant scattering alters the kernel of Eq. (4).

Resonant-scattering kernel. In the presence of the empty upper subband, the constant interaction V for electrons of the Fermi sea acquires a frequency-dependence of the form

$$\tilde{V}(\omega) = V_{12} \frac{G_2(\omega)}{1 - V_{22}G_2(\omega)} V_{21}. \quad (7)$$

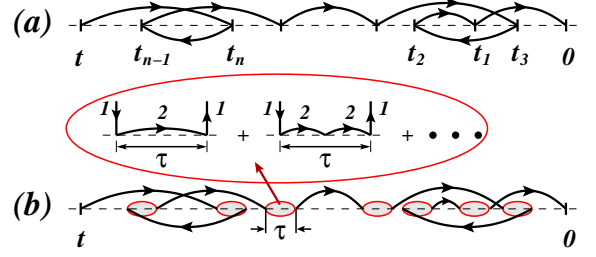


FIG. 3: (Color online) (a): Typical contribution, Eq. (6), to the transient Green function in ND theory. *Instantaneous* scatterings take place at time moments, t_1, t_2, \dots, t_n . (b): In the presence of a resonant level, each scattering act involves a "visit" to the resonant level, and takes a finite time, τ . Blowup illustrates a ladder of scatterings off the core-hole in the upper subband, 2, which lead to resonant scattering in the lower subband, 1.

Here V_{12} and V_{22} are inter- and intra-subband matrix elements of the hole potential, respectively; G_2 is the Green function of the upper subband,

$$G_2(\omega) = \sum_q \frac{1}{\omega - \epsilon_{2q} + i\eta}, \quad (8)$$

and $\epsilon_{2q} = \hbar^2 q^2 / 2m$ is the spectrum near the bottom. The form Eq. (7) is a result of summation of ladder-type diagrams, see a blowup in Fig. 3. Bound state emerges as a pole in Eq. (7),

$$E_{ex} = \frac{2\pi^2 m}{\hbar^2} |V_{22}|^2 \quad (1D), \quad E_{ex} = D e^{-\frac{2\pi\hbar^2}{m|V_{22}|}} \quad (2D). \quad (9)$$

Expanding near the pole, we simplify \tilde{V} to the form

$$\tilde{V}(\omega) = \left(\frac{\Gamma}{\pi\nu_0} \right) \frac{1}{\omega - \Delta + i\eta}, \quad (10)$$

where width, Γ , is given by

$$\Gamma = \frac{2\pi\nu_0 E_{ex}}{|V_{22}|} |V_{12}|^2 \quad (1D), \quad \Gamma = \frac{2\pi^2 \hbar^2 \nu_0 E_{ex}}{m|V_{22}|^2} |V_{12}|^2 \quad (2D). \quad (11)$$

Effective interaction Eq. (10) corresponds to *repulsion* for $\omega > \Delta$ and to *attraction* for $\omega < \Delta$. In the resonant-scattering regime, the kernel in Eq. (4) instead of the simple product $VG(\tau - \tilde{\tau})$ becomes a convolution

$$K_{res}(\tau, \tau') = \int_t^0 d\tau^* G(\tau - \tau^*) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(\tau^* - \tau')} \tilde{V}(\omega). \quad (12)$$

Integration over ω can be carried out explicitly, yielding

$$K_{res}(\tau, \tau') = i \frac{\Gamma}{\pi} \int_t^0 d\tau^* \frac{\theta(\tau^* - \tau')}{\tau - \tau^*} e^{-i\Delta(\tau^* - \tau')}. \quad (13)$$

For most interesting case, $\Delta = 0$, the expression for the kernel assumes the form

$$K_{res}(\tau, \tau') = -i \frac{\Gamma}{\pi} \ln \left| \frac{\tau}{\tau - \tau'} \right|. \quad (14)$$

We see that $\ln|\tau - \tau'|$ in K_{res} emerges in the place of $1/(\tau - \tau')$ in the ND kernel. This is a consequence of *opposite signs* of interaction with resonant level for electrons and for holes.

Derivation of Eq. (3). Substituting Eq. (14) into Eq. (4) and performing the rescaling

$$\varphi(\tau, \tau'|t, 0) = \frac{\nu_0}{t} \phi\left(\frac{\tau}{t}, \frac{\tau'}{t}\right), \quad (15)$$

we arrive to the following dimensionless equation

$$\phi(x, y) = -\frac{1}{x-y} + i\gamma \int_0^1 dz \ln\left(\frac{x}{|x-z|}\right) \phi(z, y), \quad (16)$$

where $\gamma = \frac{\Gamma}{\pi}t$. Note that the kernel Eq. (16) is much less singular than the ND kernel. As a result, the power-law transient factor in the ND solution, $[(1-x)y/(1-y)x]^{\delta/\pi}$, which is singular for $x \rightarrow 0, y \rightarrow 1$, does not emerge. This allows us to search for solution of Eq. (16) as a linear combination,

$$\phi(x, y) = \sum_n c_n(y, \gamma) u_n(x), \quad (17)$$

of the eigenfunctions, $u_n(x)$, of the Hermitian integral operator

$$\hat{R}\{u_n(x)\} = \int_0^1 dz \ln|x-z| u_n(z) = \lambda_n u_n(x), \quad (18)$$

where λ_n are the eigenvalues. The kernel in Eq. (18) is symmetric with respect to $x = 1/2$. Correspondingly, $u_n(x)$, $n = 0, 1, 2, \dots$ are even (for n even) and odd (for n odd) functions of $(x - \frac{1}{2})$. Substitution of Eq. (17) into both sides of Eq. (16) yields the following expression for coefficients of expansion,

$$c_m(y, \gamma) = \frac{a_m(y) + b_m d(y, \gamma)}{1 + i\gamma \lambda_m}, \quad (19)$$

where

$$a_m(y) = \int_0^1 dz \frac{u_m(z)}{y-z} = \lambda_m u'_m(y), \quad (20)$$

$$b_m = \int_0^1 dz u_m(z) \ln z = \lambda_m u_m(0). \quad (21)$$

In the second identities of Eqs. (20), (21) we used the properties of operator \hat{R} .

The kernel, $\ln x - \ln|x-y|$, of Eq. (16), in addition to the difference term, contains a y -independent term. As a result, b_m in the expression for $c_m(y, \gamma)$ enters with coefficient

$$d(y, \gamma) = i\gamma \int_0^1 dz \phi(z, y), \quad (22)$$

which is *the same* for all m , so that Eq. (22) can be viewed as a self-consistency condition.

Our key observation which will be justified later is that, the relevant values of m in the expansion Eq. (17) are $\gg 1$. For such m , it can be shown that eigenvalues behave as $\lambda_m \approx -1/m$. Concerning the eigenfunctions $u_m(x)$, they assume constant value near the boundaries, $u_m(0) = \pm u_m(1)$, while the derivatives, $u'_m(x)$ diverge logarithmically at the boundaries. Outside of small ($\sim 1/m$) intervals from the boundaries, they behave as $\sin(2\pi x/\lambda_m)$ and $\cos(2\pi x/\lambda_m)$. All these large- m properties can be established upon integrating by parts in Eq. (18). Then the remaining integral will be determined by a narrow domain, $|x-z| \sim 1/m$. The same simplification allows us to obtain a concise expression for $d(y, \gamma)$, namely,

$$d(y, \gamma) \simeq -i\gamma \ln(1-y), \quad (23)$$

and subsequently the solution for $\phi(x, y)$ in the form

$$\phi(x, y) \simeq -\ln(1-y) \sum_n \frac{[u_n(1) + i\gamma \lambda_n u_n(0)] u_n(x)}{1 + i\gamma \lambda_n}. \quad (24)$$

In calculating $I(\omega)$ from Eq. (24) the combination, $\sum_n u_n(1) u_n(x)$, appears. This combination is equal to $\delta(1-x)$ and does not contribute to absorption, which is determined by $x \rightarrow 0$ and $y \rightarrow 1$. In ND problem, divergences in the time domain are cut off by the inverse bandwidth, iD^{-1} . In our case, the logarithmic divergence in Eq. (24) is terminated at $(1-y) = i(E_{ext})^{-1}$. Correspondingly, the minimal x in Eq. (24) is, in fact, $x_{min} = i(E_{ext})^{-1}$. Taking this into account and using Eqs. (5) and (15), we express $I(\omega)$ in the integral form

$$I(\omega) \simeq \frac{2\nu_0 \Gamma}{\pi} \text{Im} \int_0^\infty dt e^{i\omega t} S(t) \ln(iE_{ext}t), \quad (25)$$

where the sum,

$$S(t) = \sum_{\text{odd } m} \frac{\lambda_m u_m(0) u_m(x_{min})}{\lambda_m \Gamma t + i\pi}, \quad (26)$$

is performed over only odd m , for which $u_m(1) = -u_m(0)$. Summation over m requires large- m values of $u_m(0)$. In fact, these values saturate with increasing m . This follows from the identity

$$\sum_{\text{odd } m} \lambda_m u_m(0) u_m(x) = \frac{1}{2} \ln\left(\frac{x}{1-x}\right). \quad (27)$$

The left-hand side has a logarithmic divergence at $x \rightarrow 0$. In the right-hand side, with $\lambda_m \approx -1/m$, logarithmic divergence of the sum is achieved with $u_m(x) \approx u_m(0) \approx 1$ for $m < x^{-1}$. Eq. (27) is a direct consequence of the identity, $\ln x = \sum_m \lambda_m u_m(0) u_m(x)$. The sum over odd m appears upon writing this identity for x and $(1-x)$ and taking their difference. Comparing Eqs. (26) and (27) we conclude that

$$S(t) \approx \frac{1}{4} + \frac{1}{2\pi i} \ln(i\Gamma t x_{min}) = \frac{1}{4} + \frac{1}{2\pi i} \ln\left(\frac{E_{ext}}{\Gamma}\right). \quad (28)$$

Imaginary part of $S(t)$ is determined by the upper cut-off, while $\text{Re}S(t)$ comes from $m \sim \Gamma t$; relevant values of m are large, as we assumed above. Factor Γt in the argument of the logarithm comes from the terms in sum Eq. (26) with $m \lesssim \Gamma t$.

With $S(t)$ being time-independent for $t \gg \Gamma^{-1}$, integration in Eq. (25) recovers our result Eq. (3). Physical meaning of the enhancement factor, Γ/ω , in Eq. (3) is the number of times electron virtually visits the resonant level and returns back to the lower subband during the time $1/\omega$.

Concluding remarks. (i) Our main result, Eq. (3), was obtained by setting $\Delta = 0$ in the kernel Eq. (13). Finite- Δ correction to $A(\omega)$ is small as $(\Delta/\omega)^2$. Let us briefly discuss the opposite limit, $\omega \ll |\Delta| \ll \Gamma$. In this limit, the characteristic time t in Fig. 3 is $\gg |\Delta|^{-1}$. Then, our above consideration for $\Delta = 0$ applies only in the time domain $(-|\Delta|^{-1}, 0)$. In the remaining domain $(t, -|\Delta|^{-1})$ characteristic time intervals $t_i - t_{i+1}$ in Fig. 3 are much bigger than $|\Delta|^{-1}$. This makes scattering "instantaneous", and ND theory applicable in the domain $(t, -|\Delta|^{-1})$; corresponding time-independent scattering amplitude and effective bandwidth are $\Gamma/(\pi\nu_0\Delta)$ and Δ , respectively. Separation of time scales leads to the absorption coefficient in the form of a product of $(\omega/|\Delta|)^{-2\arctan(\Gamma/\Delta)/\pi} \approx (\omega/|\Delta|)^{-\text{sign}\Delta}$ (from long times), and $\Gamma/|\Delta|$ (from short times, $|t_i| < |\Delta|^{-1}$). With shake-up included, the overall result for absorption coefficient,

$$A(\omega)|_{\Delta>0} \propto \frac{\Gamma}{\omega} \left(\frac{\omega}{\Gamma}\right)^{\frac{1}{4}}, \quad A(\omega)|_{\Delta<0} \propto \frac{\omega\Gamma}{\Delta^2} \left(\frac{\omega}{\Gamma}\right)^{\frac{1}{4}}, \quad (29)$$

is illustrated in Fig. 2. At $\omega \sim \Delta$, Eq. (29) matches Eq. (3) with logarithmic accuracy.

(ii) Ellipses in Fig. 3 can overlap; this corresponds to double-occupancy of the resonant level, which our theory does not prohibit. This implies that the Hubbard repulsion, U , is smaller than Γ . Since U is inversely proportional to the radius of the level wave function, this condition can be met.

Even more interesting is the situation when resonant level, which is split off the upper band by the core-hole, is well below the Fermi level ($|\Delta| \gg \Gamma$), and U is not small. Then the level gets occupied, and after time $\sim T_K^{-1} \sim \exp[\pi\Delta/2\Gamma]$ a Kondo peak of width $\sim T_K$ is formed at the Fermi level [17]. Photoexcited electron will experience dynamical resonant scattering from this peak. One can argue that our result for dynamical resonant scattering regime will apply in this situation, with replacement, $(\Gamma/\omega) \rightarrow (T_K/\omega)$. However, we cannot make this analogy rigorous because the Kondo scattering of the state ω leads to finite lifetime $\sim T_K/\omega^2$.

Another interesting possibility is then the core-hole possesses spin [18]. Then a Kondo peak at the Fermi level will form even without the upper subband, so that

the scattering off the core-hole will become a Kondo-scattering with ω -dependent scattering phase.

(iii) We stated above that, unlike the single-electron-line contribution, $I(\omega)$, the shake-up factor, $P(\omega) = (\omega/\Gamma)^{\arctan^2(\Gamma/\Delta)/\pi^2} \approx (\omega/\Gamma)^{1/4}$, is not sensitive to the sign of the detuning, Δ . To prove this statement rigorously, one has to extend evaluation of the many-body overlap integral Ref. [19] to the case of resonant scattering with frequency-dependent scattering amplitude $\tilde{V}(\omega)$. The modified overlap integral reads

$$-\frac{1}{(2\pi)^2} \int_0^1 d\lambda \int_{-\infty}^{\infty} d\Omega \frac{\tilde{V}(\Omega) G(\Omega)}{1 - \lambda \tilde{V}(\Omega) G(\Omega)} \times \int_{-\infty}^{\infty} d\Omega' \frac{\ln[1 - \lambda \tilde{V}(\Omega') G(\Omega')]}{(\Omega' - \Omega + i\eta)^2}. \quad (30)$$

For $\tilde{V}(\Omega) = \text{const}(\Omega)$, the integral Eq. (30) comes from small arguments, namely $\Omega \rightarrow 0^+$ and $\Omega' \rightarrow 0^-$. It diverges logarithmically with coefficient $-(\delta_0/\pi)^2$, where $\delta_0 = -\text{Arg}[1 - VG_r(0)]$, and G_r is the retarded Green function. Using the analytical properties of resonant scattering amplitude, Eq. (10), one can check that the above logarithmic divergence persists when \tilde{V} is frequency-dependent. Independence of the sign of Δ follows from the fact that coefficient in front of logarithmically divergent part is $\frac{1}{\pi^2} \delta_{\Delta}(0)\delta_{-\Delta}(0)$, where $\delta_{\Delta}(\omega) = \tan^{-1}[\Gamma/(\omega - \Delta)]$ is the resonant-scattering phase.

(iv) We neglected a contribution to absorption from a direct transition core-level $\rightarrow E_{ex}$. Since the width of E_{ex} is $\sim \Gamma$, this contribution is non-singular at small ω .

(v) Fermi edge physics manifests itself also in resonant tunneling via an impurity [20]. However, the regime $\Delta \ll \Gamma$, considered in the present paper, can not be realized in this setting since at long times impurity gets reoccupied.

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